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We have developed and applied a perturbation approach to study Bose-Einstein condensates using a full many-body Hamiltonian. Our approach offers distinct advantages for describing a large system of N interacting identical particles. In particular, our approach has the potential to yield insight into the dynamics of motion of the condensate by defining collective coordinates at first order. Our initial many-body results for a Bose-Einstein condensate indicate that very accurate many-body results are possible using powerful group theoretic techniques with a quite modest amount of computation. This method can be applied to strongly-interacting condensates which bridge the gap between dilute condensates which can be described by mean field treatments and the regime of superfluidity/superconductivity where strong interactions make first principles treatments difficult. Characterizing condensates in the strongly interacting regime where correlation effects are important is the goal of this research.

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# Final Report

The goal of our research is the formulation and application of a perturbation approach to study new $N$-body systems under quantum confinement using a full many-body Hamiltonian. These systems, such as Bose-Einstein condensates, quantum dots, and atoms confined in an optical lattice, are presenting new challenges for the many-body techniques currently available. Our method appears to offer distinct advantages for describing a large system of $N$ interacting identical particles. In particular, for Bose-Einstein condensates our perturbation approach has the potential to yield insight into the dynamics of motion of the condensate by defining collective coordinates at first order. Low-order results can thus provide simple pictures of dominant motions if the higher-order corrections are small.

Our many-body formalism, which has been published in a series of four papers, was developed specifically to handle systems with a large number of coordinates. The zeroth and first-order perturbation equations involve $N$ only as a parameter, an important simplification. We obtain an analytic formula for the zeroth-order energy which contains some correlation effects between the bosons. Not surprisingly our zeroth-order results are significantly better than Thomas-Fermi. The first-order corrections are obtained by defining normal modes of motion. The highly symmetric structure at zeroth-order greatly simplifies the determination of normal modes and fundamental frequencies which describe the dominant macroscopic motions of the condensate.

Our initial many-body results for a Bose-Einstein condensate indicated that very accurate many-body results are possible using powerful group theoretic techniques with a quite modest amount of computation. Although the Gross-Pitaevskii equation gives satisfactory agreement for existing dilute condensates, this equation will eventually breakdown as densities increase and/or the scattering length is tuned to higher values. Strongly-interacting condensates bridge the gap between dilute condensates which can be described by mean-field treatments and the regime of superfluidity/superconductivity where strong interactions make first principles treatments difficult. Characterizing condensates in the strongly interacting regime where correlation effects are important is the goal of this research.

## Approach

During the past four years my group at the University of Oklahoma has been developing an approach to solve the Bose-Einstein many-body Hamiltonian. Our approach is a perturbation approach which has been successfully used in many fields of physics[1–3] and is particularly appropriate for a system of many identical bosons since it is able to take advantage of the high degree of symmetry of the condensate. At zeroth-order, the physics and computational difficulties simplify since the derivative terms of the transformed kinetic energy drop out yielding a Thomas Fermi-like highly symmetric starting point. The first-order equation is harmonic and includes terms from both the trap and the interatomic interaction.

As an initial test of this approach we completed and published[4] a study of a simple one-dimensional Hamiltonian derived by Bohn and coworkers[5]. Our results for this simple one dimensional problem were extremely encouraging. We then applied a similar treatment[6] to the Gross-Pitaevskii(GP) equation. The lowest-order results using our dimensional perturbation treatment (DPT) were significantly better than Thomas-Fermi numbers.

The goal of these first two studies was to obtain the insight and expertise to go beyond the GP equation and study the full many-body Hamiltonian.

Dimensional perturbation theory (DPT) constitutes a conceptually different approach to including many-body effects. The perturbation is made in the kinetic energy rather than in the potential energy. This results in the correct physics at low order because the kinetic energy **is** at a minimum for a ground state condensate at $T = 0$. In our zeroth-order equation the derivative terms of the Hamiltonian drop out, but some kinetic energy is retained, namely some terms which account for the zero-point energy of the ground state. However the most important advantage obtained by using this perturbation theory is the ability to take advantage of the high degree of symmetry of a large condensate of identical bosons. The equilibrium structure that results at zeroth-order allows us to define a point group for the condensate which greatly simplifies the analysis of normal modes and fundamental frequencies at first order.

## Progress

Two years ago we completed a successful first application of a very general formalism for an $N$-particle wavefunction[7] for a Bose-Einstein condensate[8]. This powerful formalism which was developed in an earlier series of four papers(I,II,III,IV)[9–12] uses group theoretic techniques to take full advantage of the symmetry of the condensate at low order. In the zeroth and first-order perturbation terms, $N$ enters only as a simple parameter, an important simplification.

We formulated the first-order results by defining the normal modes which are allowed for the $N$-body system of bosons and solved for the harmonic frequencies using the GF matrix method of Wilson, Decius and Cross[13].

We were able to drastically simplify the reduction of the FG matrix by taking advantage of the high degree of symmetry which exists at zeroth-order. The atoms at zeroth-order are frozen in a highly-symmetric, high-dimensional tetrahedron in which every atom is equidistant from every other atom. We define symmetry elements (i.e. high dimensional reflections and rotations) and thus determine a point group for this structure. The FG matrix, which could potentially have dimensions of $M^2$ where $M = N(N+1)/2$, block diagonalizes into small (1x1 and 2x2) matrices most of which are highly degenerate. As an expression of this degeneracy, the FG matrix yields analytical formulas for five fundamental frequencies of oscillation at first-order. Note that there are only five (!) normal modes for a condensate in a symmetric trap.

Our results for the ground state of a very strongly interacting condensate fall between the Gross-Pitaevskii results and the modified Gross-Pitaevskii(MGP) results which are thought to be a little high. The excitation frequencies which provide a sensitive test of many-body effects show particularly large shifts from mean field results[8].

## Conclusions

At the present time we have perhaps the most advantageous method of studying condensates beyond the mean-field approximation. Our method is accurate, numerically robust, and it brings in the important physics at low order yielding physical pictures of dominant modes of oscillations. We are currently extending this work on several fronts.

While our initial results go up to 10,000 atoms, a considerable achievement for a fully interacting calculation, many condensates today have $10^7$ bosons. Our present results indicate that as the number of atoms increases, it will be necessary to include higher order terms in the perturbation series.

Knowledge of the normal modes enables us to construct the Jacobian weighted wave function which will be a product of harmonic oscillator functions for each normal mode.

This wavefunction will then allow us to calculate any quantity of interest e.g. expectation values, transition matrix elements, and density profiles, the probability of finding an atom at a given radius. This quantity which is automatically produced in quantum Monte Carlo calculations is desirable to obtain since it is experimentally accessible. An undergraduate who has recently signed up with my group is planning to work on the determination of the condensate wavefunction.

A careful study of the higher excitation spectrum is planned, initially at harmonic (first) order. Eventually this effort could require bringing in higher order terms in the perturbation expansion, a major undertaking which we have recently started. We're particularly interested in analyzing the transition from collective excitations in which the entire condensate oscillates to single particle excitations. This transition could shed light on the dynamics behind superfluidity/superconductivity since single particle transitions result in the loss of coherence.

A major goal of the research is the development and application of the formalism using a cylindrical trap. Initially our formalism assumed that the magnetic trap set up to contain the bosons was symmetric. This results in the highest possible symmetry and the lowest number of dominant excitation modes. Our development of the formalism using a cylindrical trap indicates that this extension will result in a very interesting modification of the spherical trap modes due to the reduction in symmetry. More importantly, we are still able to obtain analytic results through first order with $N$ as a simple parameter despite the reduced symmetry. Studying these excitation modes is certainly highly desirable in order to connect with results from experiments which use almost exclusively cylindrical traps. Our analysis should reveal new excitation modes for the cylindrical trap that can be verified experimentally and should connect with the experiments which use a Feshbach resonance to tune the interaction strengths to large values.

The results of our many-body perturbation approach for a BEC in a symmetric trap demonstrates that this method treats Bose-Einstein condensates in a very advantageous way. Our results for strongly-interacting condensates are compelling. The extensive use of the symmetry properties of the condensates makes the calculations fairly simple numerically since much of the real work is done on paper. Thus, we expect our method to remain robust for larger condensates which have millions of two body interactions. The excitation modes yield insight into possible oscillation behavior that has not been observed yet. We are currently working on the extension of our results to larger condensates, the calculation of a wavefunction for the condensate, and the analysis of the normal modes. Our extension to cylindrical traps will allow us to connect to experimental results. We expect that this interaction with experiments will both open up new projects and guide the future direction of this work.

We are optimistic that the group theoretic techniques of our general many-body formalism will be able to treat the many-body effects of any large system of particles under quantum confinement and will yield insight into the microscopic basis for the properties of such systems which have the potential for important technological advances.

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